CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

No. 20 April 1985

WHAT IS CACHE?

CACHE is a non-profit organization whose purpose is to promote cooperation among universities, industry, and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960's, the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, 14 chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. Initially, the CACHE Committee was sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers, including both educators and industrial members, and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its on-going projects. Information on CACHE activities is regularly disseminated through **CACHE News**, which is published twice each year. Individual inquiries should be addressed to:

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CACHE TRUSTEES

CACHE NEWS

The **CACHE News** is published two times a year to report news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by D.M. Himmelblau with contributions from a number of CACHE members and representatives.

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TASK FORCE FOR LARGE-SCALE SYSTEMS

Dr. Jeffrey Siirola (Eastman Kodak) was recently appointed chairman of the CACHE Large-Scale Systems Task Force. J.D. Seader (University of Utah) will continue to manage what had been the principal work of the task force, the preparation and distribution of FLOWTRAN load modules for chemical engineering departments to install on their own in-house computers.

The Large-Scale Systems Task Force is now considering embarking on a number of new projects in the areas of process synthesis, alternative simulators (for example, suitable for microcomputer implementation), and simulator enhancements. The first project is being directed by Professor Lorenz Biegler and is expected to employ the infeasible path method. This enhancement and an accompanying new chapter for the FLOWTRAN manual should be available next year.

PROCESS DESIGN CASE STUDIES

by Ignacio Grossmann
Carnegie-Mellon University

The first volume of the CACHE Process Design Case Studies is now available for distribution. This case study is on "Separation System for Recovery of Ethylene and Light Products from Naphtha Pyrolysis Gas Stream." The design problem deals with the synthesis of the process flowsheet and the detailed analysis for economic evaluation.

This case study consists of three parts: material for the instructor, preliminary design calculations by hand, and an extensive design report. The problem statement was supplied by Dr. Dan Maisel from Exxon Chemicals, and the project was performed at Carnegie-Mellon University. The case study should be helpful to instructors of the undergraduate design course since it contains all the relevant information on the design problem, and it presents approaches and solutions for the synthesis and analysis of the flowsheet.

The price for CACHE-member departments is $10 for the first copy (handling fee) and $35 for each additional copy. The price for departments which are not members of CACHE is $35 per copy. An order form for the case study is located at the end of this newsletter and should be sent to Professor Brice Carnahan at the University of Michigan.

Two other case studies are under preparation: "Design of Ammonia Synthesis Plant" and "Production of Acataldehyde by Dehydrogenation of Ethanol." These reports should be available by the end of the summer. Problem statements are also available on "Alcohol Isolation System" and "Solvent Recovery System," supplied by Dr. Jeffrey Siirola from Eastman Kodak. For information on these design problems, or for anybody interested in submitting a design report, please contact:

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CACHE MICROCOMPUTER/PERSONAL COMPUTER NOTES

Edited by Peter R. Rony
Virginia Polytechnic Institute & State University

In a series of reports in his February/March 1985 newsletter (DTACK GROUNDED, 1415 E. McFadden, Ste. F, Santa Ana, CA 92705), editor Felgercarb N. Eloi made the following observations: (a) He received two 68020 samples at $610 each in January 1985; they run at 12.5 MHz and have a "wart list as is usual for initial samples of such complex parts;" he expects initial production of 68020 in the summer of 1985. (b) Hitachi and Thompson CSF, a French company, do not have available 16 MHz 68000 parts. (c) Advanced Micro Devices is now producing some 10 MHz 80186 processors. (d) There has been no publicity recently about the Intel 80386; he predicts that nobody will get their hands on this part until 1986. (e) He guesses that "nobody is going to hold a Z80000 in his hand this year. Besides, the Z80000 is limited to 64K linear addressing, like Intel's 80286." (f) Motorola has working parts of the 68881 math chip and is selectively sampling them to large customers. "The good news is that the 68881 is reported to be very fast, especially on transcendentals. The bad news is that it appears to be best suited for use with the 68020, not the 68000."

Summary evaluations of leading business computer programs and a listing of the most popular applications software are contained on pages 117-124 of the December 1984 issue of **Business Computer Systems**, which is circulated without charge to qualified subscribers (Cahners Publishing Company, 221 Columbus Ave., Boston, MA02116). TK!Solver is the fifth largest selling spreadsheet, after Miltiplan, FlashCalc, VisiCalc, and SuperCalc3. Bank Street Writer and PFS:Write are the top two word processors. Popular packages in the miscellaneous category are Dollars & Sense, Chart, Sensible Speller, Microsoft Project, SpellStar, PFS: Proof, Harvard Project Manager, and Desk Organizer.

Byte's special issue on communications (December 1984) features articles on "The Evolution of a Standard Ethernet," "Local-Area Networks for the IBM PC," "High-Speed Dial-Up Modems," "Writing Communications in BASIC," "Looking for the Perfect [Communications] Program," and "The On-Line Search." The Zenith Z-150, Tandy Model 2000, Word Perfect, and TK!Solver are reviewed in the same issue.

The February 1985 issue of **Byte** (page 42) contained a short announcement that caught our fancy: "Satellite Broadcast Network has announced a satellite service that will transmit financial and news information to personal computer owners. You will need a 12-GHz satellite-receive antenna, a low-noise amplifier, a solid-state receiver, and SBN's demodulator; all are available from SBN for $695. SBN will also charge a fee for access to each type of information, starting at about $25 per month. SBN will use multiple 9600-bps channels." Contact Satellite Business Network, Inc., 212 West Superior St., Chicago, IL 60610. The low cost for the antenna and associated hardware indicates that this type of technology will impact all of us before too long.

The February 1985 issue of **Byte** also contains the following: (a) "Simulate a Servo System," an article and seventy-line BASIC program that might be useful for disbelieving undergraduates in our controls courses. (b) "Interfacing for Data Acquisition," which discusses the IEEE-488 interface in some detail. A BASIC data-acquisition routine using the IEEE-488 interface is provided. (c) A review of two Modula-2 compilers.

Apple's new laser printer is described in the February 1985 issue of **MACWORLD** (PC World Communications, Inc., 555 De Haro St., San Francisco, CA 94107), certainly the slickest computer magazine available today. See "The Laser's Edge," pp. 70-79. The pictures make one drool, but for $6995 you can get more than a lifetime's supply of napkins.

In "Battle of the Boards" (**Datamation,** January 1, 1985), Willie Schatz predicts that "the enhancement board [for the IBM PC] business is going to be reduced to two or three major players." Key companies include Tecmar, AST Research, Quadram Corp., and Hercules Computer Technology.

"DEC Puts VAX on Eight ICs" (Datamation, February 1, 1985) predicts that a desktop version of the 11/780 supermini is coming from DEC next year, with a price that is 70% less. "But the ink was hardly dry on the MicroVAX II before talk emerged of a 1.22 million-transistor/chip MicroVAX III, allegedly already in silicon...The MicroVAX III is believed to have an I/O capability equal to DEC's line-topping Venus, some 13.3 MBps." DEC has been having a rough time in the competitive personal computer market lately.

Recent computer buzzwords are RISC (reduced instruction set computer) and CISC (complex instruction set computer). Read the article, "RISC-Y Business?" in the February 15, 1985 issue of **Datamation** for insight into important developments and perspectives concerning RISCs.

Dr. Dobb's Journal (December 1984) is a special UNIX issue that is worth reading. Articles include "Varieties of UNIX," "UNIX Device Drivers," and "A UNIX Internals Bibliography." A UNIX family tree is given on page 35.

APL*PLUS/PC (Version 3.1) is reviewed in the January 1985 issue of **Dr. Dobb's Journal**. The review mentions an excellent comparison between APL*PLUS/PC (Version 2.6) and IBM APL (Version 1.00) that appeared in the March 1984 issue of **Byte**. Also reviewed or discussed in this issue are VSI—Virtual Screen Interface (Version 2.09), which "is a programmer's tool kit for building applications that manipulate the PC's screen to take advantage of overlapping windows and features such as color and borders," and PCDOS (Version 3.0). The February 1985 issue of Dr. Dobb's reviews Module—2/86 (Version 1.04).

McGraw-Hill's **Electronics Week,** the successor to the biweekly **Electronics** magazine, contains information that permits one to predict near-term trends in silicon products. "Cell Library Shelved on Large-Scale ICs" (December 3, 1984) discusses the exciting topic of "standard-cell libraries—those complete electronic functions that a user can design into an application-specific integrated circuit." While such libraries have been available for SSI and MSI functions (flip-flops, op amps, and memories, for example), recently a new wave of jumbo cells have surfaced. Waferscale Integration Inc. has just "introduced what it says is the first U.S.-made large-scale cell, an implementation of the popular 2901 bit-slice microprocessor." Such developments point to the further reduction of a full board of chips to a single chip that contains all of the individual chip functions as standard cells.

In **Electronics Week** (December 10, 1984), Sytek Corp.'s move to license PC Network protocols is discussed. PC Network is based on Sytek's Local 20, " a product that is a carrier-sense, multiple-access local-network system with collision detection operating at 2 MB/s on coaxial cable. IBM licensed the protocols from Sytek for use with PC Network." "For $5000, Sytek will license the description of its protocols and the protocol specifications with which other firms will be able to build products that would be compatible with IBM's network..." IBM's objective is to dominate the local network market as it does the personal computer market. An important competitor is Ethernet, which currently has 2000 installations.

The December 17, 1985 issue of **Electronics Week** continues its attention on local area networks (LAN) with two brief discussions, "Two Low-Speed Nets Race to Link

Computers'' and ''Unique Net Links MACs with IBM PCs.'' The first is on AT&T's 1-Mb/s and 2-Mb/s local-area networks, which are vying for selection by the IEEE as standard for personal computers. The second is on the Transcendental Networking System, which can link computers of different makes and operating systems, such as the IBM PC, Apple Macintosh, and UNIX- and CP/M-oriented microcomputers; the networking system is known as Tops. The dust should settle in the LAN area within several years.

Speaking of jumbo cells, the January 1, 1985 issue of **Electronics Week** describes a Toshiba CMOS super-integration chip that is in development. It contains a Z-80 processor and three other large blocks: a counter/timer, a programmable peripheral interface, and programmable I/O. It is another example of the reduction of a small board of chips to a single superchip.

The actual and predicted sales of 256K dynamic random access memory (DRAM) circuits are staggering. According to ''DRAM Makers Gird for 256-K'' (**Electronics Week**, January 14, 1985), ''Fujitsu Ltd. already claims to be shipping 2.5 million units a month, while NEC Corp. and Hitachi Ltd. are believed to be shipping at near the same rate.'' ''Deliveries are likely to peak in 1989, with forecasts calling on commercial shipments ranging from 2 billion to over 3 billion chips.'' Unbelievable! Also mentioned is the ''traditional 70% drop in bit costs per year'' and the expectation for ''prices on 256-K chips to swoop down to $9.50 each by summer.'' 64-K DRAMs currently sell for $1.60 each in quantity (**Electronics Week**, February 11, 1985, p. 19).

A significant product announcement appeared in the February 11, 1985 issue of **Electronics Week**. ''Super Cube,'' which is based upon the Caltech Cosmic Cube, now becomes Intel's 'personal supercomputer' and brings megaflops-range processing within reach of more individuals. Called the iPSC, the product contains 32, 64 or 128 nodes, each node containing an 80286 CPU, 80287 math coprocessor, 512-Kbytes of CMOS DRAM, and 64-Kbytes of ROM. Interested? Prices are expected to range from $150,000 to $500,000. When one considers the history of how prices of computer hardware decrease, 2.5 to 10 Mflops of computing power should be on your desktop by 1990 for under $20,000 (1990 dollars).

''DSP Chips Spark Lackluster Market'' (**Electronics Week**, February 11, 1985) describes new developments in digital signal processor (DSP) chips. There is a nice figure that relates the number of arithmetic operations/second to specific applications: digital control, guidance, speech synthesis, speech vocoding, modems, speech recognition, hi-fi audio, robotics and vision, and imaging. Scheduled for end-of-the-year introduction is Texas Instruments, Inc. new 32-bit DSP chip, which bears the code name Shiva, after the Hindu god of destruction and reproduction. ''Digital signal-processing is fundamentally different from mainstream data processing in that real-world analog inputs are typically digitized and then mathematically manipulated on the fly through a series of fast multiplications and summations. Processing architectures and instruction sets are often tailored to quicken the execution of polynomials used in complex algorithms for self-adaptive filters. In a sense, a DSP can be considered a RISC with its instructions highly optimized for signal processing.''

''LAN chips will soon rival microprocessors in strategic importance,'' says Dave House, vice-president of Intel Corporation (**Electronics Week**, February 11, 1985, pp. 26-27). ''House says that microprocessors are running out of gas in terms of complexity, and that the 32-bit design is likely to prove to be a practical limit. Even the Cray Systems, Inc. supercomputer, he points out, uses a 32-bit instruction. 'The next level of growth will come from tying personal computers together, so that we go from making individuals more productive to making organizations more productive, ' House says.'' We agree. If the 1970s can be considered to be the decade of the personal computer, then the 1980s will be considered as the decade of the computer network.

An important new product is the Intel 27916 KEPROM, which is described on page 73 of **Electronics Week** (February 11, 1985). What is a KEPROM? It is a Keyed-access erasable programmable read-only memory; it is used to prevent unauthorized copying of ROM-stored system software. ''Gaining access to stored code in a system that contains a 27916 KEPROM entails an authentication handshake procedure. The handshake requires two KEPROMs to communicate with each other—over telephone lines or directly over a bus on a processor board—according to a two-way verification protocol.'' The handshake routine is as follows: ''1. KEPROM 2 generates random number. 2. Random number is written to KEPROM 1. 3. KEPROM 1 encrypts number. 4. Encrypted number is written to KEPROM 2. 5. KEPROM 2 compares this value with original random number. 6. If there is a match, KEPROMs reverse roles and repeat handshake routine.''

IEEE Spectrum (January 1985) is a special issue on Technology '85. Experts review developments in minis and mainframes, personal computers, software, microprocessors, communication, solid state, instrumentation, industrial electronics, power and energy, consumer electronics, transportation, aerospace and military, and medical electronics. We would be fortunate if CEP had one-hundredth the quality of **IEEE Spectrum**—truly one of the fine magazines of engineering.

The December 1984 issue of **Mini-Micro Systems** has a number of interesting brief articles. For example: (a) On page 37, it is stated that ''IBM PCs now are the leading resident on engineers' desktops.'' According to Dr. Joel N. Orr, ''The PCs are cheap compared with Digital Equipment Corp. and Hewlett-Packard Co. products, and they are ubiquitous." Two articles briefly discuss different IBM PC Engineering/Scientific (PC/ES) workstations. (b) Digital Research, Inc. will market a Macintosh-like interface to MS-DOS. It is called the Graphics Environment Manager (GEM), which replaces MS-DOS commands and utilities by icons such as disks and trash cans and by pull-down menus. Companion software products include the GEM Desktop, GEM Programmer's Toolkit, GEM Draw, and GEM Wordchart. The products should appear sometime in 1985. (c) "New DECmate and Professional Computers Receive Lukewarm Welcome" (pp. 54-59) discusses the problems that DEC is having at the low end of its computer line. (d) "Third-party Developers Concerned Over IBM Microcomputer Software" (pp. 62-63) has a lovely figure that summarizes "IBM's 31 flavors of software." (e) "Will IBM Personal Computers Set a New Hardware Bus Standard" (page 75). The bottom line seems to be as follows: "With IBM's market power and its complete control over the operating system, CPU and motherboard configuration, the computer industry may find itself endorsing one of the few standards not subject to any standards-setting group's approval." In the world of IBM, seemingly nothing changes. (f) "Operating Systems Conform to Application Needs." Nice article by James F. Ready (Hunter Ready, Inc.) who knows this subject inside and out. Sidebars discuss how operating systems handle application tasks, and how semaphores, mailboxes, and monitors prevent resource contention. (g) "Protocol Converters Link Incompatible Devices." At Virginia Tech, we use a protocol converter to interface a Z89 personal computer as a RJE terminal to an IBM mainframe. (h) "Teaching Computers English Proves Easier Than Training People." On the subject of natural languages. NOTE: **Mini-Micro Systems** is circulated without charge to qualified readers. Write to Cahners Publishing Company, 221 Columbus Avenue, Boston MA 02116.

The January 1985 issue of **Mini-Micro Systems** contains the following articles: (a) "Enhancement Programs Add Features to IBM PC Operating System, Application Software." Discusses shell packages—which provide an envelope (or sleeve) around the operating system—and application add-ons. (b) "Network Software Bridges Gap Between Local Area Networks." Novell Inc.'s NetWare file-server operating system has been ported to 18 major LANs for IBM PC/XTs, ATs, and compatibles. The LANs include Omninet, ARCnet, G-Net, S-Net, proNET, PLAN 2000, EtherLink, PCnet, and MultiLink. Such LANs indicate the degree of competition (and confusion) that currently exists in the area. A conservative strategy would involve the selection of a LAN, a standard, from a company that is likely to remain in the field after the dust settles. (c) "Printer Manufacturers Elbow for Shelf Space." Discussion of what is happening in the printer market.

In the February 1985 issue of **Mini-Micro Systems**: (a) "Networks 1.0 Provides IBM Compatibility." Networks 1.0 is Microsoft's new software that is compatible with IBM's networking scheme. The software runs under the new MS-DOS 3.1 operating system. Microsoft claims it will also run under IBM's PC-DOS 3.1, expected to be available the first quarter. (b) UNIX Emerges as a Universal Tool Kit" (pp. 149-175). A useful article that includes an extensive directory of operating system.

From **PC World** magazine comes the following articles: (a) "Six Leading LANs" (February 1985, pp. 108-128). The networks that are compared include Netware/S-Net, EtherSeries, Omninet, PLAN 3000, PCnet, and Net/One. (b) "Word Processing: The Deciding Factors" (March 1985, pp. 53-57). The article states: "More than 200 word processing programs crowd the market. Some are easy to use but limited in functions; others can do almost anything but take weeks to master." With his inability to remember—after a week spent at out-of-town meetings—ten different commands for each of seven different software packages, your friendly editor prefers a simple word processor.

PC Tech Journal tends to go into nitty gritty details more than does **PC World** or **PC**. If you like assembly language debuggers, consider "Entymological Explorations" (January 1985, pp. 88-105). The same issue has "Kermit" (pp. 110-123) and "The Limited Joys of Translated Software" (pp. 143-146). Kermit is a general-purpose file-transfer protocol that was developed on college campuses (see the September 1984 **CACHE News** MC/PC Notes for additional references).

The December 1984 issue of **Systems & Software** discusses the IBM XT/370 in "XT 370 Pushes IBM Plan to Link All Products Via VM/CMS" (pp. 63-66).

STATUS OF FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

by J.D. Seader
University of Utah

As part of a continuing program of support to education Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to departments of chemical engineering to install on their own in-house computers. Thus departments would be able to run FLOWTRAN on their own computers at no charge other than that of their own computer center. CACHE is continuing the supervision of the preparation of FLOWTRAN load modules for a wide variety of main-frame, supermini, and supermicro-type digital compters and the distribution of the modules on magnetic tape to those departments that order them. Instructional books on FLOWTRAN are already available through CACHE by using the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

1. **DEC VAX 11-7XX** series of super minicomputers running with the VMS operating system.
2. **DEC 20XX** mainframe computer running with the FORTRAN-20, Version 7 compiler (9-track, 1600 BPI tape).
3. **UNIVAC 1100** series computers running under the EXEC 1100 (38R2/08) operating system with the FORTRAN 77-SID (10R/A) compiler (9-track, 1600 BPI tape).
4. **Amdahl** computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).
5. **IBM** AND IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and 43XX with the following operating system and FORTRAN compiler combinations:

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	0S1/MVS	IV-H ext
c	OS/VS2 MVS	VS
d	CMS	IV-G1

6. **IBM PC-XT-370** personal compter operating in conjunction with an IBM mainframe.
7. **CDC Cyber** mainframe computers with the NOS operating system and a FORTRAN V compiler.

Conversions are also underway for the Apollo DOMAIN, DEC 10, Honeywell, Sperry 90/80, Data General MV/8000, DEC VAX under UNIX, and Prime machines. Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes, but not for consulting. A total of 94 FLOWTRAN tapes have already been distributed to departments at the following universities for the computers indicated:

Univ. of Adelaide	DEC VAX 11-780
Univ. of Akron	IBM 370/158
Univ. of Arizona	DEC VAX 11-750
Arizona State Univ.	IBM 3081, IBM 4341/62, IBM PC-XT/370
Univ. di Bologna	DEC VAX 11-780
Brigham Young Univ.	DEC VAX 11-750
Univ. of British Columbia	Amdahl 470
Bucknell Univ.	Apollo DOMAIN
UC, Berkeley	IBM 3081/K32
UC, Davis	DEC VAX 11-780
UC, San Diego	DEC VAX 11-780
Calif. State Poly., Pomona	CYBER 170-750
Carnegie-Mellon Univ.	DEC VAX 11-780
Case Western	DEC 2060
Colorado School of Mines	DEC VAX 11-750
Univ. of Colorado	DEC VAX 11-780
Columbia Univ.	DEC 2060
Univ. Concepcion (Chile)	DEC VAX 11-780
Univ. of Connecticut	IBM 3081D
Cooper Union	DEC VAX 11-780
Cornell Univ.	IBM 4341
Univ. of Delaware	DEC VAX 11-780
Drexel Univ.	IBM 3081
Ecole Poly.	IBM 4341
Florida Inst. Tech.	DEC VAX 11-780
Florida State Univ.	DEC VAX 11-750
Georgia Tech	DEC VAX 11-750
Univ. of Houston	DEC VAX 11-780
Howard Univ.	IBM 3033S
Illinois Inst. of Tech.	DEC VAX 11-780
Univ. Illinois at Chicago	IBM 3081D
Iowa State	DEC VAX 11-780, NAS AS/6
Kansas State	NAS 6630
Univ. of Kuwait	Univ.AC 1100-62
Lehigh Univ.	CYBER 170-730
Univ. Southwestern Louisiana	DEC VAX 11-750
Louisiana State Univ.	IBM 3081
Louisiana Tech	IBM 370
Lowell Univ.	DEC VAX 11-780
Manhattan College	DEC VAX 11-780
Univ. of Massachusetts	DEC VAX 11-780
McMaster Univ.	DEC VAX 11-780
Univ. of Michigan	Amdahl 5860
Michigan State	Amdahl 5860
Michigan Tech. Univ.	UNIVAC 1100-80A
Mississippi State	UNIVAC 1100-80A
Univ. Nacional del Sur (Argentina)	DEC VAX 11-780
Univ. of Nebraska	DEC VAX 11-780
New Jersey Inst. Tech.	DEC VAX 11-780, Sperry 90/80-4
New Mexico State	DEC VAX 11-780
New South Wales (Australia)	DEC VAX 11-780
CC-CUNY	DEC VAX 11-750, IBM 4341
North Carolina State	IBM 3081
Northeastern Univ.	DEC VAX 11-780, DG MV/8000
Univ. of Notre Dame	Prime 850
Tech. Univ. of Nova Scotia	DEC VAX 11-780
Oregon State Univ.	CDC CYBER
Univ. of Ottawa	Amdahl 470-A
Univ. of Pennsylvania	Univ.AC 1100

Univ. di Pisa (Italy)	IBM 3081
Pratt Inst.	DEC VAX 11-780
Univ. of Puerto Rico	IBM 4341
Purdue Univ.	CDC 6500
Rensselaer Poly. Inst.	IBM 3033
Rice Univ.	DEC VAX 11-780
Rose-Hulman	DEC VAX 11-780
Royal Military College of Canada	Honeywell DP39
Rutgers Univ.	NAS AS/9000
San Jose State	IBM 4341
Univ. of Saskatchewan	DEC VAX 11-780
Univ. de Sherbrooke	NAS 5000 E
Univ. of South Alabama	IBM 4341
Univ. of South Florida	DEC VAX 11-750
Stevens Inst. of Tech.	DEC VAX 11-780
Syracuse Univ.	IBM 4341
Texas Tech	IBM 3033
Tuskegee Inst.	DEC VAX 11-750
Univ. of Utah	Univ.AC 1100
Villanova Univ.	DEC VAX 11-780
Univ. of Washington	DEC VAX 11-750, CYBER 170-750
Washington Univ.	DEC VAX 11-750
Wayne State Univ.	Amdahl V-8
West Virginia Tech	Amdahl 470
Univ. of Wisconsin	UNIVAC 1100, DEC VAX 11-785
Worcester Poly.	DEC 2060

If you would like to obtain a FLOWTRAN tape for your computer and have not already expressed that desire to CACHE, complete and submit the form, FLOWTRAN TAPE, at the end of this newsletter. You will be required to sign a User's Agreement that must be approved by Monsanto. The cost of the tape, payable to CACHE, is $250. However, the charge to CACHE-supporting departments listed near the end of this newsletter is only $175.

GREAT PLAINS TOPICAL REPORTS

by Irven H. Rinard

The Halcon SD Group, as part of its work for the U.S. Department of Energy on the Great Plains ASPEN Model Development Project, has completed a series of nineteen topical reports describing the various aspects of the work. The Great Plains Plant, located in North Dakota, converts indigenous lignite into substitute natural gas. It is now in the final stages of startup.

Flowsheet models for eleven sections of the plant were developed. These are:

1. Oxygen Plant
2. Gasifier Quench, Cooling, Shift, and Gas Liquor Separation
3. Rectisol Plant
4. Methanol Synthesis
5. Methanation Section
6. Gas Compression and Drying
7. Phenosolvan Unit
8. Phosam Section
9. Stretford Sulfur Recovery
10. Steam Generation and Distribution
11. Cooling Tower

The other reports cover physical properties screening and modeling, cost and sizing evaluation and enhancement, and the selection and incorporation into ASPEN of a moving-bed gasifier model. There is also an Executive Summary report.

It is felt that some of the flowsheet models may be of interest for process simulation or design courses. For further information, contact Irven Rinard at 212-689-3000.

THIRD INTERNATIONAL CONFERENCE ON CHEMICAL PROCESS CONTROL

The third Conference (CPC-III), sponsored by CAST, NSF & CACHE, will be held January 12-17, 1986, at the Asilomar Conference Grounds in California. It will focus on advances that have taken place in the process control field over the last five years. In particular, developments in control system robustness, process operability, adaptive control, and model predictive control will be highlighted. On-line identification and optimization, reactor control, and actual industrial applications of advanced control will be discussed. Finally, the potential impact of artificial intelligence and new educational approaches will be assessed. All conference sessions will be held mornings and evenings, leaving afternoons for recreational activities and ad hoc discussion groups. To encourage active participation and discussion, the number of attendees will be limited with selection made on the basis of their involvement in the field of process control. You must apply for attendance by June 15, 1985. Applicants will be informed by August 15, 1985 of selection for participation in CPC-III. An application form is located at the end of this newsletter.

ABOUT THE FIRST TWO CONFERENCES

The first Chemical Process Control Conference (CPC-I) was held in Asilomar, California in 1976 and the second (CPC-II) in Sea Island, Georgia in 1981. Both Conferences were sponsored by the AIChE and NSF and they brought together participants from industry, government, and universities to discuss and critique the current state of process control. Twelve foreign countries were represented by participants in the first two Conferences. These meetings have come to be regarded as milestones in the process control field. They have not only served to highlight recent developments, but they have had a decisive impact on research efforts in the succeeding years. They have helped to narrow the gap between process control theory and application.

LOCATION OF THE CONFERENCE
The Conference will be held at the Asilomar Conference Center, a unit of the California State Park System, in Pacific Grove, California. Situated on the tip of the Monterey Peninsula overlooking the Pacific Ocean, Asilomar occupies 105 secluded acres of forest and dune. Attractions of the Peninsula, such as Fishermen's Wharf and the newly-opened Monterey Bay Aquarium, are minutes away. Monterey is a short flight from San Francisco, Los Angeles, and San Jose; and Asilomar is 15 minutes by car from Monterey.

ACCOMMODATIONS
Arrangements have been made for single- and double-room accommodations available on the Asilomar grounds. The single-occupancy rates range from $37 to $83 per night and the double-occupancy rate ranges from $32 to $43 per night per person. All rates are under the American Plan which includes dinner, breakfast, and lunch with 3 p.m. arrival and 12 noon check-out. (Lodges with multi-bed units are available for those desiring larger accommodations.) Accommodations are also available in nearby Monterey, Carmel, and Pacific Grove.

CONFERENCE PROGRAM (Tentative)
Each session will feature two to three invited speakers. The following sessions are currently planned:

I. **Control in the Presence of Model Uncertainty**

Chairman: J. Kantor (Notre Dame University)

Speakers: J. Doyle (Caltech/Honeywell)
M. Morari (Caltech)

II. **Industrial View of Advanced Process Control**

Chairman: O. Asbjornsen (University of Houston)

Speakers: J. Doss (Tennessee Eastman)
M. Juba/J. Hamer (Kodak)

III. **Model Predictive Control**

Chairman: D. Seborg (University of California, Santa Barbara)

Speakers: C. Garcia (Shell Development)
C. Brosilow (Case Western Reserve University)

IV. **Process Operability**

Chairman: I. Rinard (Halcon)

Speakers: Y. Arkun (RPI)
T. Marlin (Exxon)

V. **Adaptive Control**

Chairman: E. Ydstie (University of Massachusetts)

Speakers: K. Astrom (Lund)
G. Dumont (University of British Columbia)

VI. **Identification and On-Line Optimization**

Chairman: T. Edgar (University of Texas, Austin)

Speakers: G. Goodwin (University of Newcastle)
M. Morshedi (Shell Oil)
T. Baker (Numetrix Decision Sciences)

VII. **Reactor Control**

Chairman: W.H. Ray (University of Wisconsin)

Speakers: D. Gilles (University of Stuttgart)
G. N. Stephanopoulos (Caltech)
K. Jensen (University of Minnesota)
D. Schnelle (DuPont)
J. Richards (DuPont)

VIII. **Speculations on the Future of Process Control**

Chairman: G. Stephanopoulos (MIT)

Speakers: T. Umeda (Chiyoda)
J. Taylor (General Electric)

IX. **Reflections by an Industrial Practitioner**

Speaker: F.G. Shinskey (Foxboro)

For the afternoons informal presentations of process control design software are planned.

SPEED COMPARISONS OF PC'S AND VAX'S

by Alan T. Moffet
Robinson Laboratory of Astrophysics
California Institute of Technology

I have made some comparisons of the computing speed of various PC's and of two models of the Digital Equipment VAX, and I thought these might be of general interest to their users.

No single number can be used to compare the speed of two different computers, since their performance will depend on the mix of different types of instructions in the test program and on the efficiency of code generated by the compilers used. The first part of this statement is true even when comparing the same object code run on two members of the same computer family, such as the VAX 11/780 and the 11/750. The largest differences may arise when one is equipped with floating-point hardware and the other is not, but there are other more subtle differences between models.

To show how the instruction mix affects performance, I have used five benchmark programs. Their characteristics are as follows.

SIEVE — strictly integer and logical instructions,
NINTSUM — solid double-precision floating-point arithmetic,
FOURD — double-precision Fourier series,
FFTRUN — single-precision FFT's--probably the best approximation to a typical data analysis job, and
SAVAGE — solid double-precision transcendental function calls.

Two of these, SIEVE and SAVAGE, have been run on a very wide variety of computers, from an HP-15 to a Cray (see **Byte**, Jan. 1983 and **Dr. Dobb's Journal**, September 1983 and August 1984). Keith Shortridge, at Caltech, wrote the VAX versions of SIEVE.

The run times, in elapsed time for the PC's, which run only one job at a time, and in CPU seconds for the VAX's, are given in Table I. Run times for the PC's will vary somewhat with the number of device drivers installed, since these add to system overhead. I have included the new IBM AT, which uses the 80286/80287 combination, as well as the older IBM XT and Zenith Z-100, which use the 8088/8087 combination. IBM "clones", such as the Compaq and the Zenith Z-150, should have the same performance as the XT. The tremendous effect of the 8087 floating-point processor is shown by including one line of results from a Z-100 without an 8087. An IBM PC without an 8087 would give slightly longer run times.

The effect of compiler efficiency can be seen by comparison of the same programs run on each machine in FORTRAN and C. For the case of SIEVE there are also run times for an optimized assembly-language version of the program. One can see that the VAX compilers come within 20-30% of the best that can be done with carefully written assembly language, while the microcomputer compilers are notably less efficient. This is probably because the 8088 or 80286 registers are so few in number and specialized in their use that a compiler can't take advantage of them as a programmer working in assembly-language can. For instance, register-type variables are not supported in Lattice C on the PC's.

The Lattice C compiler (Version 2.12) was delivered with a library of floating-point functions which was so bad that the Caltech educational computing project had to commission an undergraduate to write a better one, the J2 library mentioned in Table 1. (This improved the C performance on SAVAGE by a factor of 150!)

The new IBM Professional FORTRAN compiler has about the same performance as the older Microsoft FORTRAN compiler (or IBM PC FORTRAN Version 2.0), however it is a complete implementation of ANSII FORTRAN 77, which makes it easier to transport programs from the VAX to the PC. Floating-point function calls are handled very efficiently, so the performance of the new compiler on FOURD and SAVAGE is significantly better.

Table 2 is an attempt to express the speed of several types of hardware relative to the VAX 11/780 on different sorts of problems. One can see the strong effect of the floating-point hardware in both the VAX and the microcomputer. The higher speed of the 80286 in the AT, relative to the 8088 in the other PC's, is apparent only on integer and logical operations; for floating-point operations the 80287 in the AT is clocked at 4 MHz, while the 8087 in the XT runs at 4.77 MHz. A faster 80287 is promised at some future date.

None of these numbers reflects the speed of compilation and other operations where the disk data transfer rate is the dominant factor. Nevertheless, it is a remarkable measure of progress in computing technology that a $3000 computer will deliver something like a tenth of the power of a $250,000 11/780. (A more nostalgic comparison is that the same $3000 machine has very nearly the scientific computing power of an IBM 7090, which cost about $500,000 in 1964.)

Table 1

Run times in CPU seconds

Language/ Machine	FPP	SIEVE	NINTSUM	FOURD	FFTRUN	SAVAGE
VMS FORTRAN						
VAX 11/780	FPA	1.44	1.99	2.54	1.29	1.16
VAX 11/750	FPA	2.40	2.93	3.79	1.94	1.85
VAX 11/750	none	2.55	15.18	10.65	4.22	7.97
VMS C						
VAX 11/780	FPA	1.21	1.50	2.91		1.52
VAX 11/750	FPA	2.05	2.11	4.29		2.44
VAX 11/750	none	2.11	12.28	10.81		8.65
MS-FORTRAN						
AT	80287	6.26	29.39	12.05	19.90	6.15
XT	8087	19.60	26.97	12.41	26.64	6.48
Z-100	8087	18.37	26.13	11.60	22.92	6.18
Z-100	none	18.37	527	383	378	248
IBM Professional FORTRAN						
AT	80287	7.91	33.23	8.57	23.89	4.23

Lattice C with J2 library					
AT	80287	3.46	68.52	11.85	4.62
XT	8087	10.95	112.9	17.65	4.95
Z-100	8087	10.14	107.3	15.26	4.57
Assembly					
VAX 11/780	—	1.06			
VAX 11/750	—	1.93			
AT	—	1.49			
XT	—	4.04			
Z-100	—	3.74			

Table 2

Comparison of Computing Power Relative to VAX 11/780

Type of Problem	XT 8087	AT 80287	11/750 no FPA/FPA
Integer and logical, optimized	.26	.71	.55
Integer and logical, compiled	.11	.35	.57
Single-precision scientific	.05	.06	.31/.66
Double-precision math	.07	.07	.16/.70
Double-precision transcendentals	.25	.25	.15/.64

DEVELOPING A MICROCOMPUTER-BASED DATA-ACQUISITION SYSTEM

by David R. Wynne
Cincinnati — ESPC

ABSTRACT

Microcomputers are now becoming a widely-used tool in the Chemical Process Industry primarily due to the low cost.

This paper presents a case study containing methods and techniques used to design and program an Apple II + computer to form a Data-Acquisition System. Along with descriptions of procedures used on the actual project, there are explanations of general procedures to follow on any project which involves real-time interfacing of a computer with a production process.

ABOUT THE AUTHOR

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INTRODUCTION

The use of microcomputers in the Chemical Process Industry is becoming increasingly common as memory and peripherals expand while prices decrease. Computers now are more than just a design tool; they are finding uses in industrial environments. While digital control systems can be purchased specifically for process control, home and personal business computers are being used as aids to manufacturing and process automation.

One important use of the microcomputer is as a Data-Acquisition System. This can provide timely and concise feedback on process conditions, equipment performance or product quality which can be translated into dollars saved, increased productivity, and a better understanding of the process [1].

We recently undertook the task of making a real-time data acquisition and analysis system from an Apple II + computer. Our system was designed to do the following:

1. Take data at periodic intervals for 2 asynchronous batch processes.
2. Monitor control switch for batch running status (start-stop).
3. Present a menu of control options and accept input from the operator.
4. Perform statistical analysis of the data (mean and standard deviation).
5. Print analysis report for each batch.
6. Print report at end of day for each process showing daily trends.
7. Store data on disk for further analysis.

All this was to be done at low cost and as quickly as possible, using an off-the-shelf microcomputer and peripherals. Operator interface had to be user-friendly and system reliability was important.

The following article explains the methodology used to design and build the data acquisition system.

DEFINITION

The initial phase of a project is the project definition. This is where the requirements of the system are specified and documented. This phase should cover the following areas:

A. Define the overall scope of the project.
B. Determine exactly what the finished product is to do.
C. Decide which materials are to be used, including computer hardware, cables and testing equipment.
D. Define how the system will operate.
E. Develop a preliminary workplan and schedule.

The overall scope of the project should include specifying and buying hardware, design and coding of software, testing and debugging equipment and procedures, and a list of required documentation.

In deciding what you want the system to do, carefully examine the process to find what data is available, how often and from what sources. Next, determine exactly what it is you need to know and whether your data sources can provide you with sufficient information for your desired output. From this, you can determine what it is you want the system to do and a good design will determine how this will be done.

In our case, the process consisted of two asynchronous batch processes with six data points each. The desired output was two types of reports; a summary for each batch and a daily report showing trends of batch parameters. Additional data required for reports were not available from the process and would have to be entered by the operator.

Next was the hardware decision and justification. The hardware specification was made early in the project so that it could be purchased and delivered in time for coding and debugging. Two main factors were involved in hardware selection: 1) existing software and 2) memory and interfacing capabilities of the computer. The existing data recorder had available software for interfacing with several different microcomputers. From this list of micros we selected the Apple II + because it had sufficient capacity for the job and because of ease of programming (past Apple experience). A list of hardware is presented in Table 1.

Table 1
Hardware List

1 Apple II + computer
1 Apple Monitor with Coaxial Cable
2 Apple Disk Drives with Control Card and Cables
1 Epson MX-80 Printer with Cable
1 32k Microbuffer Card
1 16k Memory Expansion Card
1 Apple Super Serial Card
1 Clock Card (Mountain Computer, Inc.)
1 RS-232-C Compatible Cable (Data Logger to Serial Card)
1 8-Wire Ribbon Cable (Game I/O Port)
1 Custom Cabinet to House System

After it was determined what the system would do and what materials would be used, we could determine how the system would operate. This encompasses how to incorporate the system into the existing process and how to interface with the operator.

Our project was to be a turnkey system. It would connect to the data logger through a serial line and the serial interface card (see Installation Section) and would receive data upon request. The batch run status would be obtained by monitoring the existing process On/Off switches. The game I/O port was available for 2 state (on/off) inputs and outputs. This port was used to read the switches and output clicks and beeps for various key inputs.

All operator inputs were through the keyboard. Visual feedback was provided through the video monitor. The screen was divided into three areas (see Figure 1). The top of the screen provided status information for quick review. The center portion was the data entry section which provided prompts and echoed the operator responses. The bottom of the screen displayed a menu of options available from the current location in the program. Other outputs went to the printer for hardcopy records or to the data disk for later analysis.

Figure 1 Sample - MONITOR DISPLAY

```
STATUS - PROCESS 1                    STATUS - PROCESS 2
              <<SYSTEM BUSY MESSAGE>>
**** TITLE OR DESCRIPTION OF ENTRIES TO BE MADE ****
====================================================

                 DATA ENTRY SECTION

  ENTRY                                  OPERATOR
  PROMPTS                                RESPONSES

----------------------------------------------------

                   MENU SELECTIONS
```

A complete list of physical inputs and outputs was created at this time. From this list, a partial data I/O list was created which showed which data variables were needed in different phases of the program and helped provide groundwork for the programming phase.

Finally, a schedule was developed based upon the predicted plant start-up date. Hardware was ordered first in anticipation of extended delivery times on some items and software development time was estimated based on the completed project definition.

DESIGN

Once you complete the project definition, the next step is to design the system. This is a critical phase and should not be cut short or bypassed, as time spent here will almost certainly be saved in later phases.

Our data acquisition system was designed to operate as follows:

—The computer would scan process On/Off switches periodically

a. the switch determined batch status (start, suspend, restart, end, abort)
b. a one-line batch status report was sent to the printer with every switch change
c. the current batch status was displayed at the top of the screen for each process

—Data readings would be taken via a serial line connection from the data logger at regular intervals. These intervals would be unique for each process and would start from the time the switch was turned to ON position. A final reading would be taken when the batch was ended.

—Ending a batch would cause a batch summary report to be prepared and printed featuring Mean, Standard Deviation, High Value and Low Value for each data element being examined.

—The operator would be able to Abort a batch through keyboard entry which would delete all previously-collected data for that batch.

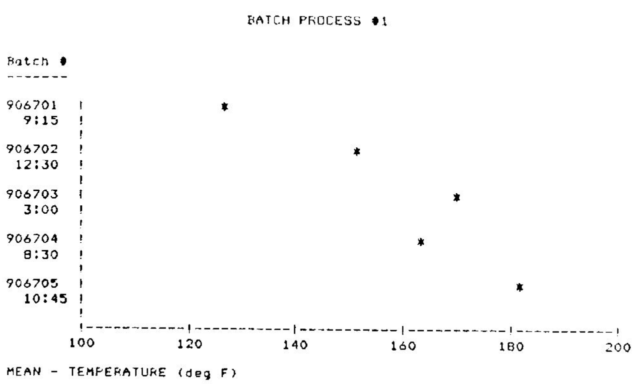
—Utility options could be called from a separate menu at the end of the day. This would be independent for each process. Options were:

a. store data on disk and assign a file title containing the process number, date and number of batches in the file
b. print daily report containing plots of daily trends (see Figure 2)
c. reinitialize data arrays (this would be done automatically after the report was printed)

—Display a <SYSTEM BUSY> message while taking data or writing to disk and keyboard was unresponsive.

—Allow for easy changes of input data elements to be analyzed.

Figure 2 Sample - DAILY REPORT



All this was to be done in a real-time environment on a menu-driven system. This meant user-friendliness, which can turn simple software into a programmer's nightmare. In anticipation of dealing with unskilled operators, the system was designed to accept only proper input keys, ask for verification, provide menus for all entry options and always allow the user to change an input. The system was to operate in the same fashion as an automatic bank teller.

PROGRAMMING

If a thorough system design is done, programming your software should be a simple process of transferring your design to code. Such is not often the case, however, and programming becomes a mess of patchwork as redesign ends up being done on the fly.

We decided to go with BASIC language, since it comes with the APPLE and could most likely be maintained by someone other than the programmer. BASIC is not a "structured" language and tends to form long, convoluted programs.

One of the most important techniques used in programming the software was MODULARITY. This technique involves writing the program as a series of small routines instead of one long one. There are several advantages to this method. One is that you can avoid duplicate sections of code by taking operations which are performed more than once and placing each in a separate subroutine which can be called from anywhere in the program. Another is clarity. Each individual operation is performed in its own section of code, making the flow of logic easier to follow. Testing is also made easier by debugging each module before integrating it with the rest of the program.

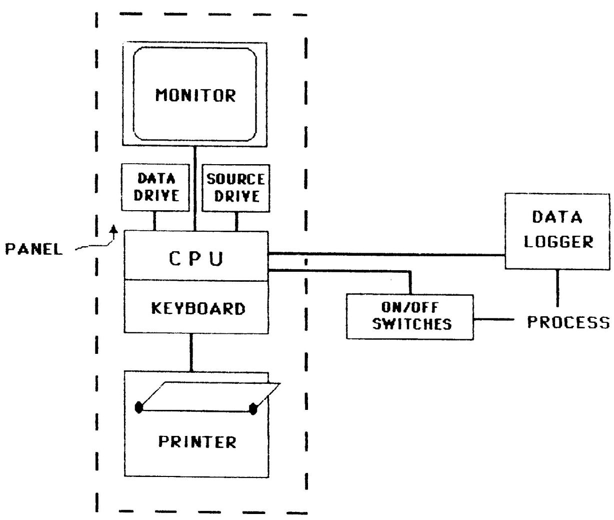
Including comments in program code may be a nusiance while coding but is necessary and greatly appreciated by anyone trying to follow your program. The main benefactor of well-commented code, however, is often the programmer himself. When it comes time to debug a long and involved routine, nothing is more welcome than a brief description of what variables are being used and what is being accomplished in each section of code.

The final phase of programming is Simulation. This may often involve resoursefulness on the part of the programmer for he must convince the computer that it is really connected to an active process. For our system, we hard-wired switches to the game I/O port to imitate On/Off switches. The input from the data logger was simulated through software which involved writing and debugging a separate simulation routine. Unfortunately, certain sections of the communications software could not be tested in this environment and had to be debugged during installation.

INSTALLATION

The physical location of the computer was to be on the process floor where the operator would have easy access to it. An enclosed cabinet was fabricated to house the system and was purged with air to ensure safety (see Figure 3 for a System Diagram). Another advantage to having the computer on the process floor was that RS-232 cable could be used to form the serial link with the data logger. The serial interface was the only significant problem encountered during start-up and could have been avoided by having a data logger available during the program simulation phase.

Figure 3 SYSTEM DIAGRAM



The On/Off switches were then connected through a terminal to the game I/O port and the rest of the system was reconnected as it had been in the programming phase.

The final phase of installation was Operator Training. This involved demonstration and review of the User's Manual to give the operators an understanding of the purpose and capacities of the new system. The system was designed for use with minimal keyboard skills and menu-driven to keep learning time to a minimum. The operators were surprisingly receptive to the new system which may be a reflection of the growing acceptance of personal computers in today's society.

DOCUMENTATION

As with all projects, good documentation is important. Yet most people will tend to put it off as long as possible. Don't wait until the end of the project to start preparing your documentation. "Documentation and training are not left until last in successful projects. Documentation should go on continually, in case a programmer suddenly leaves" [2].

Our project produced essentially 5 documents. These were:

1. System Definition Document
2. System Design Document
3. Systems Manual
4. User's Manual
5. Remarks within the Code itself

The Definition Document was produced at the end of the Project Definition Phase and stated exactly what the system would and would not do. The Design Document was produced at the end of the System Design Phase and explained exactly how the system would work. The Systems Manual was written at the close of the project and contained everything needed to maintain and update the program including a listing of the code. The User's Manual was completed before Installation and provided the end user with a detailed description of how to operate the system. Finally, the code itself contained enough remarks that someone could follow the logic without much difficulty.

CONCLUSION

Microcomputers are now becoming a widely-used tool in the Chemical Process Industry. "The primary motivation is low cost." The data-acquisition system's immediate payoff was in providing fast analyses and a well-organized database of process information. It also saved operators from shuffling through reams of datalogger paper.

In the long term, data analysis is expected to lead to a better understanding of the process, and better process performance.

Points to be stressed when building any microcomputer system are a thorough design and well-documented code. Any shortcuts in either of these facets will quite likely lead to unnecessary confusion and rework before your system has been put to use.

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SOFTWARE SERVICES FOR THE CHEMICAL, PETROCHEMICAL AND PLASTICS INDUSTRY

The utility of computer simulation, computer aided analysis, design and control is well established in every facet of industrial activity. However, the industrial user requires "ready to use" programs that can provide reliable results, readily with no excessive effort on his part, and no need for excessive adaptation to problems of interest.

Existing commercial facilities already cater effectively in the fields of standard (steady state) process simulation, project management, accounting, inventory control and the like. Many other specialized aspects of great importance to the industrial user in R&D, engineering or production have been developed over the years in the Department of Chemical Engineering at the Technion—Israel Institute of Technology and are now made available to external users.

Information on various programs follow. (Some are programs from the open literature which were enhanced and made interactive.) Most programs can be made available to academic institutions at cost of mailing and handling.

APPLICATIONS PROGRAMS

Engineering Programs

Material and Energy Balance Simulator (MEBAL)
Allows fast evaluation of material and energy balances for process flow sheets while avoiding detailed computation of processing units. Includes an option for separate evaluation of material balances.

Stream analysis, identification of recycles, computation ordering and loop tearing. Easily formulated inputs. Wide choice of processing units. Simplified input for material balance runs. Reliable convergence of iterative computations. Admits 50 processing units, 100 streams, up to 9 inlet and outlet streams per unit, up to 50 chemical compounds in each stream. Physical properties library for 400 compounds.

Dynamic Simulator of Processes and Their Control (DYSIM)
Real time dynamic simulation of a process, interactively defined, allowing the involvement of the operator at all times. Suitable for continuous, deterministic processes. Contains nonlinear arithmetic operators. Interactive programming using prepared forms. Possibility of operating with live (real) systems.

Data Acquisition and Analysis of Continuous Signals (DAD)
Data gathering from continuous signals. Acquisition, graphic display and filtering.

1) Operating capacity of 16 signals.
2) Data structure fits the Control Lab's standard and allows the transfer to/from other programs.

Notes: 1) Interactive program.
2) Recorded signals must be in the range 0-5 VDC.
3) Fastest sample rate for a single channel is about 1 KHz.

Simulation of Multi-Component Distillation (DIST82)
Computation of distillation column with ideal stages where equilibrium constants are a function of component fractions.

At each stage it is possible to introduce feed or to allow exit of a liquid, vapour or mixed stream, and to add or remove heat. There is no limit on the size of the problem. There are various options in calculating equilibria by a method based on the Redlich-Kwong equation or by the UNIFAC method.

Distillation Program (HANSON 1)
Computes distillation column for given feed and operating conditions. It is possible to specify recoveries and the program will set reflux ratio or distillate flow (as required) accordingly.

Accepts up to 20 components, 100 stages and 3 feeds. Apart from simulation, allows for a certain level of design. Improvements have been made in the original program. The main difficulty is in the definition of the required correlations for equilibrium constants and for enthalpy. Additional programs which accept correlations of a given form and convert them to the required form by regression are available.

Shortcut, Rapid Computation of Distillation Column (SHORT)
The program uses the accepted approximation methods such as that of Fenske, Underwood and Gilliland to calculate the number of stages, recycle ration and feed plate.

The user has a choice between two methods to calculate the number of minimum stages and five methods to determine the number of stages. The user can opt for defaults.

Simulation of Multicomponent Extraction (BENO)
The program computes concentration profiles and recovery in staged extraction column. The column accepts recycle and feed at all stages, and it is possible to remove side streams from any phase at any stage, in addition to the exits at each end. The program has had proven performance for industrial systems.

The program is very efficient and flexible. Failure only occurs if poor equilibrium coefficients are provided.

Extraction Program (HANSON 2)
The program calculates flow and concentration profiles in a staged extraction column and recoveries for given column inlet conditions. It is also possible to specify required recovery of a given component at the top of the column and the program will manipulate the solvent flow rate in order to obtain this recovery, if possible, by only varying this parameter.

The program is very efficient for small problems. Side stream exits are not allowed. Programming errors were removed from the original program as found in the literature. In addition, internal generation of an initial guess was added, input was simplified and output was improved.

Liquid-Liquid Shell and Tube Heat Exchanger (HEATEX)
The program carries out optimization of yearly costs taking into account the price of the heat exchanger, the cost of pumping and the value of the heating or cooling fluid. Allows for choice of shell fluid. It is possible to define practical limits to velocities and temperatures. The pressure drop

is calculated. The program has not yet been tested on an industrial system, but is more advanced than in the referred paper.

Synthesis of a Heat Exchanger Network (HENET)
The program carries out the optimization of a system of heat exchangers between various hot and cold streams. The energy balance is completed by cooling water, cooling air, steam generation, steam heating or furnace accordingly in order to reduce overall costs.

The program includes the complete design of all types of heat exchangers, and cooling and heating equipment, not using the simplistic method usually employed in the literature in the treatment of this problem. Because of the large number of possible combinations, the cost of computation rises sharply with the size of the problem.

Single Screw Extruder Simulator (EXTRUDE)
The computer program simulates the extrusion process from the hopper to the die. It incorporates a collection of mathematical models dealing with conveying of solids, melting, mixing and pumping and their interactions. It can handle a variety of mixing sections.

Coat Hanger Die Simulator (DIEDES)
The program simulates the optimal geometry of coat hanger dies, specifically the manifold design for uniform film or sheet thickness. An isothermal non-Newtonian flow model is used. Both tubular and elliptical manifold designs can be handled. In existing dies, cross sheet straining for settings are computed.

Injection Mold Design Program (INJECT)
The program simulates with a simplified finite element numerical technique the flow of polymer melt into injection molds. The program can handle multiple gates. The flow is isothermal, the fluid non-Newtonian.

Process Control Programs

Process Analysis and Control Evaluation (PACE)
This is a very powerful, graphical interactive multi-levelled tool providing for the thorough analysis of processes described by systems of differential and algebraic equations, including parametric testing of the steady state, characteristic dynamics about desired steady states, observability and controllability, root locus testing, relative gains testing, parametric investigation of proportional control system.

1) Suitable for deterministic, continuous processes.
2) Can successfully handle non-linear processes.

Notes: 1) Interactive operation involves the user with decision-making over the entire length of the computation, like a programmed discussion.
2) The graphic output matches and strengthens the user intuition.
3) The user should have a basic working knowledge of the APL language.

Process Identification and Frequency Domain Analysis (IDENT)
Discrete time domain signals are transported to the frequency domain by Fourier transform. Formulation of transfer functions in frequency domain from pairs of measured signals.

1) Can accept up to 5 signals.
2) Data structure fits the Control Lab's standard and allows the transfer of data to/from other programs.
3) The program is interactive.

Frequency Domain Analysis and Control System Synthesis (FACTS)
Generation of frequency response from given transfer functions. Graphic display of Bode and Nyquist diagrams. Fitting transfer fuction to the frequency response generated by identification. Has successfully dealt with linear systems up to 10th order with dead time. The program is interactive.

System Designer's Interactive Tool (SYSDIT)
Fits rational transfer function to a file of frequency domain identification data. Allows for the analysis of feedback systems in the frequency domain.

Work with the program is absolutely interactive, allowing for the user's involvement at all stages of the analysis.

Frequency Response of Transfer Functions (FRESP)
Calculates frequency response of rational transfer function.

The program FACTS is significantly broader in scope and is easier to use than FRESP. The advantage of FRESP is that it can be used on any terminal.

Auto and Cross Correlation of Sampled Signals (CORREL)
Performs auto-correlation and cross-correlation of sampled signals.

Linear Systems Analysis (BASMAT)
Calculates for $x = Ax + Bu$ the functions:

1) det A
2) A^{-1}
3) $\Phi(s)$
4) $\Lambda(A)$
5) exp[At]

Rational Time Domain Response (RTRESP)
Calculates for $x = Ax + Bu$; $u = K(r - kx)$ and $y = Cx$:

$$y(t) = \sum_i^n a_i e^{\lambda_i t}$$

Graphical Time Domain Response (GTRESP)
Calculates for $x = Ax + Bu$; $u = K(r - kx)$ and $y = Cx$: the paths u(t), y(t) and x(t), and prints the results.

Root Locus Diagram (RTLOC)
Calculates and graphs the roots of the equation:

$$1 + KG(s) = 0$$

as a function of the feedback gain K where G(s) is a rational transfer function.

Root Sensitivity to Parameter Changes (SENSIT)
Calculates, for $x = Ax + Bu$ and $u = K(r\text{-}kx)$, the location of the roots of the characteristic equation of the closed loop with changes in A,B,K and k.

Observability and Controllability Test (OBSERV)
Calculates the observability coefficient of $x = Ax + Bu$; $y = Cx$.

Luenberger Observer (LUEN)
Design of a Luenberger state observer for a given system.

State Variable Feedback (SVFDBK)
Translates the time domain model: $x = Ax + Bu$, $y = Cx$ to the transfer function G(s). In addition, given the feedback law: $u = K(r - kx)$, calculates the transfer function of the closed loop and of the equivalent feedback. Limited to controllable systems.

Optimal Feedback Control (RICATI)
Calculates the optimal feedback gain matrix according to quadratic target function of state variables and control forces.

Thermodynamic Programs

Calculation of Physical Properties of a Single Component (SPOC)
The program calculates critical data, heat of evaporation at the boiling point or any other temperature, vapour pressure and specific heat from minimal data. The program uses different estimation methods depending on the type of data. Computation routes are chosen to maximize accuracy.

Calculation of Binary Margules Equation Coefficients for Use in Distillation and Extraction Programs (MARGUL)
Calculates binary Margules equation coefficients and their functional dependence on temperature from experimental data:

1) TXY for constant pressure.
2) PXY for constant temperature.
3) XY for unknown temperature and pressure.
4) Partial solubility data.

Calculation of Margules Coefficients from Liquid-Liquid Data (MARGULL)
The program calculates all the binary Margules coefficients from liquid-liquid equilbrium data for tertiary and quaternary systems.

Engineering Economics Program

Estimation of Investment and Economic Project Evaluation (INVEST)
The program calculates investment from general flow stream information and from minimal information on overhead costs, estimates the feasibility of the investment. The product price can be calculated for given profit, or the profit margin when an estimate of the price is given.

Scientific Program

Propagation of Change-of-Phase Moving Fronts (QF)
The program uses the Isotherm Migration Method to follow the moving front and to calculate temperature profiles in one-dimensional problems with a fixed-temperature boundary condition and with a melting/freezing temperature initial condition in Cartesian, cylindrical or spherical coordinates.

Propagation of Change-of-Phase Moving Fronts - 2 (QFT)
The program uses the Modified Isotherm Migration Method to follow a moving front and to calculate temperature profiles in one-dimensional problems with a radiation-type (heat transfer coefficient) boundary condition and a fusion/freezing temperature initial condition. There are three members in this library - CY for cylindrical coordinates, SL for Cartesian coodinates and SP for spherical coordinates.

Propagation of Change-of-Phase Moving Fronts - 3 (DQF)
The program uses the Modified Isotherm Migration Method to follow moving fronts and to calculate temperature profiles in one-dimensional problems with a radiation-type (heat transfer coefficient) boundary condition and any given initial temperature profile. DQF is a library with three members — CY for problems in cylindrical coordinates, SL for Cartesian coordinates, and SP for spherical coordinates.

Mathematical Programs

Mathematics Library in FORTRAN (MATLIB)
Collection of general mathematical routines in FORTRAN. All the routines can be easily called by FORTRAN programs written to run on the PDP-11/34.

Curve Fitting of Two Variables (EQSEL)
Utilizes least squares to fit the best out of 12 alternatives from a set of data for one variable as a function of another. Does not require programming knowledge. Partial overlapping with EQCOR. Limited to 100 pairs of values for x and y. No limitation on zero value. Skips zero values if causes computation problems.

Curve Fitting of Two Variables — 2 (EQCOR)
Performs a least squares fit of data to any of a choice of 36 functions. The amount of data is limited to 100 pairs. All values must be positive in order to eliminate errors due to square root or other function.

Graphics Packages

Graphics Library (PLOTLIB)
Drawing graphs on linear axes with desired scaling. Up to 6 graphs per page. The subroutines can be used to draw graphs within user-written programs.

Input and Output of Graphical Data (GIP)
Input of graphical data using digitizer which reads coordinates from the original plot and thus transfers the data to the computer. Graphical display of the result.

1) Input point-by-point or continuous.
2) Views from various angles in multi-dimensional bodies.
3) Option of entering data with various systems of coordinates.
4) Option of integrating under the curve.

Notes: 1) Does not require experience in programming.
2) Auxiliary program is available to prepare data file for other processing programs such as DAD, FACTS, etc.

Graphical Display of Data and Function Fitting (FPLOT)
Graphical display of data together with continuous polynomial function which approximates it by least squares on required coordinate scale (linear, logarithmic, half-logarithmic).

1) Requires minimal knowledge of the APL language.
2) A number of curves may be drawn on the same axis.
3) The fitted polynomial can be up to 9th order.

Graphics Executed on Printer (PLOTC)
Crossplotting of variable groups vs. a selected variable in a number table. Ordering variables according to descending value of independent variables. May stretch or reduce graph size. Includes horizontal and vertical lines as desired in graph. Specially useful to detect extraneous results. Maximum 10 variables with 200 values each. Zero value in any element voids an entire row unless replaced by a number greater than 2×10^{-5}. May choose absolute or relative scale. Must know sufficient FORTRAN to write MAIN program.

Curve Fitting and Plotting (FIT)
The program performs a least squares fit of discrete data pairs to a polynomial of order up to 6. The fit can be obtained in linear, log-log, or half-log coordinate systems thus making it possible to fit exponential functions. The results can be examined graphically and an analysis of variance and table of residuals are tabulated.

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Editors:
Arthur Westerberg
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